

Large- q Expansion of the Specific Heat for the Two-dimensional q -state Potts Model

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Abstract

We have calculated the large- q expansion for the specific heat at the phase transition point in the two-dimensional q -state Potts model to the 23rd order in $1/\sqrt{q}$ using the finite lattice method. The obtained series allows us to give highly convergent estimates of the specific heat for $q > 4$ on the first order transition point. The result confirm us the correctness of the conjecture by Bhattacharya *et al.* on the asymptotic behavior of the specific heat for $q \rightarrow 4_+$.

The q -state Potts model on the square lattice has a first order phase transition for $q > 4$. The phase transition point and many quantities at the transition point are known exactly, including the free energy, the internal energy[1] and the correlation length[2]. On the other hand, important quantities such as the specific heat and the susceptibility are not solved exactly. The correlation length increases to infinity as $q \rightarrow 4_+$, so it becomes very difficult in general to evaluate the quantities that are not solved exactly for q as ‘small’ as 5, where the correlation length reaches as large as several thousands.

Here we concentrate on the specific heat at the transition point. Many methods have been used to evaluate it including the Monte Carlo simulations[3], the low-(and high-)temperature expansion[4], and the large- q expansion[5], among which the large- q expansion appears very promising. Bhattacharya *et al.* calculated the large- q series for the specific heat and higher energy cumulants to order 10 in $z \equiv 1/\sqrt{q}$. Making the Padé analysis of the series assuming the asymptotic form in the limit of $q \rightarrow 4_+$, they obtained very precise values of the specific heat for $q \geq 7$, whose accuracy seems to be higher than the Monte Carlo simulations.

In this paper we will enlarge the large- q series for the specific heat at the transition point to order 23 in z . We use the finite lattice method[6, 7, 8], which has been used mainly to generate the low- and high-temperature series in statistical systems and the strong coupling series in lattice gauge theory. The method can give in general longer series than those generated by the graphical method in lower space (and time) dimensions. In the graphical method, one has to list up all the relevant diagrams and count the number they appear. In the finite lattice method we can skip the job and reduce the main work to the calculation of the expansion of the partition function for a series of finite size lattices, which can be done using the straightforward site-by-site integration[9] without the graphical technique.

The model is defined by the partition function

$$Z = \sum_{\{s_i\}} \exp(-\beta H), \quad H = - \sum_{\langle i,j \rangle} \delta_{s_i, s_j}, \quad (1)$$

where $\langle i, j \rangle$ represents the pair of nearest neighbor sites and $s_i = 1, 2, \dots, q$. The phase transition point β_t is given by $\exp(\beta_t) - 1 = \sqrt{q}$. We will consider the free energy density in the disordered phase, which is given by

$$F(\beta)_d = \lim_{L_x, L_y \rightarrow \infty} (L_x L_y)^{-1} \ln Z(L_x, L_y), \quad (2)$$

where the partition function for the $L_x \times L_y$ lattice should be calculated with the free boundary condition corresponding to the disordered phase. The large- q expansion of the partition function can be given through the Fortuin-Kasteleyn representation[10] as

$$Z(L_x, L_y) = q^{L_x L_y} \sum_{l,j} N_{l,j} (e^\beta - 1)^l q^{-j}$$

$$= q^{L_x L_y} \sum_{l,j} N_{l,j} Y^l z^{2j-l}, \quad (3)$$

where $N_{l,j}$ is the number of configurations of l bonds connecting the nearest neighbor sites on the $L_x \times L_y$ lattice with $L_x L_y - j$ independent clusters of sites and $Y \equiv (e^\beta - 1)/\sqrt{q}$. (Two sites connected to each other belong to the same cluster.)

We define $H(l_x, l_y)$ for each $l_x \times l_y$ lattice ($l_x, l_y = 1, 2, 3, \dots$) as[8]

$$H(l_x, l_y) = \ln [Z(l_x, l_y)/q^{l_x l_y}], \quad (4)$$

where $Z(l_x, l_y)$ is the partition function with the free boundary condition, and define $W(l_x, l_y)$ recursively as

$$\begin{aligned} W(l_x, l_y) &= H(l_x, l_y) \\ &- \sum_{l'_x \leq l_x, l'_y \leq l_y}^{(')} (l_x - l'_x + 1)(l_y - l'_y + 1) W(l'_x, l'_y). \end{aligned} \quad (5)$$

Here the $(')$ indicates that a term with $l'_x = l_x$ and $l'_y = l_y$ should be excluded in the summation. Then the free energy density defined by Eq.(2) is given by

$$F(\beta)_d = \ln (q) + \sum_{l_x, l_y} W(l_x, l_y). \quad (6)$$

We can prove [8] that the Taylor expansion of the $W(l_x, l_y)$ with respect to z and Y includes the contribution from all the clusters of polymers in the standard cluster expansion that can be embedded into the $l_x \times l_y$ lattice but cannot be embedded into any of its rectangular sub-lattices. Each cluster that contributes to the lowest order term of the $W(l_x, l_y)$ consists of a single polymer and it has the order of $z^{l_x + l_y - 2}$. An example of such a single polymer is shown in Fig. 1. Therefore to obtain the series to order z^N we have only to take into account all the rectangular lattices that satisfy $l_x + l_y - 2 \leq N$. If we set $Y = 1 + y$ [11], then we have only to keep the expansion with respect to y to order y^n to obtain the n -th energy cumulant at the phase transition point as,

$$F_d^{(n)} = \left. \frac{d^n}{d\beta^n} F(\beta)_d \right|_{\beta=\beta_t} = \sum_m a_m^{(n)} z^m. \quad (7)$$

(We note that $\frac{d}{d\beta} = (1 + y + z) \frac{d}{dy}$ and $y = 0$ at $\beta = \beta_t$.) We can also calculate the series for the energy cumulant $F_o^{(n)}$ at β_t in the ordered phase by using the duality relation

$$F_d^{(2)} - F_o^{(2)} = -z[F_d^{(1)} - F_o^{(1)}]. \quad (8)$$

We have calculated the series to order $N = 23$ in z for $n = 0, 1$ and 2 . The obtained series for the zeroth and first cumulants (i.e. the free energy and the

internal energy) agree with the expansion of the exactly known expressions. The series for the second cumulants are listed in Table 1. The coefficients for $F_o^{(2)}$ agree with those by Bhattacharya *et al.* to order 10.

The latent heat \mathcal{L} is known[1] to vanish at $q \rightarrow 4_+$ as

$$\mathcal{L} \sim 3\pi x^{-1/2}, \quad (9)$$

with $x = \exp(\pi^2/2\theta)$ and $2 \cosh \theta = \sqrt{q}$. Bhattacharya *et al.*[12] made the conjecture that $F_{d,o}^{(2)}$ will diverge at $q \rightarrow 4_+$ as

$$F_{d,o}^{(2)} \sim \alpha x. \quad (10)$$

The constant α should be common for the ordered and disordered phases from Eqs. (8) and (9). Here we follow this conjecture, then the product $F^{(2)}\mathcal{L}^2$ can be expected to be a smooth function of θ , so we apply the Padé approximation to this quantity as

$$\begin{aligned} F_d^{(2)}\mathcal{L}^2 &= zP_M(z)/Q_L(z) + O(z^{M+L+2}), \\ F_o^{(2)}\mathcal{L}^2 &= z^2R_M(z)/S_L(z) + O(z^{M+L+3}), \end{aligned} \quad (11)$$

where $P_M(z)$ and $Q_L(z)$ ($R_M(z)$ and $S_L(z)$) are the M -th and L -th order polynomials with $M+L+1 \leq N$ ($M+L+2 \leq N$). We give in Table 2 the values of the specific heat $C_{d,o}$ evaluated from these Padé approximants for some values of q and present in Fig. 2 the behavior of the ratio of the $F^{(2)}$ to x plotted versus θ . The averages and errors are taken from all the $[M,L]$ Padé approximants with $M \geq 8$ and $L \geq 8$, excluding that whose denominator has zero at some point in $4 < q < \infty$. We have checked that the duality relation (8), which is not respected exactly by the Padé approximants, is really satisfied within the accuracy for all the range of $q > 4$. These estimates are more precise by three or four orders of magnitude than (and of course consistent with) the previous result for $q \geq 7$ from the large- q expansion to order z^{10} by Bhattacharya *et al.*[5] and the result for $q = 10, 15, 20$ from the Monte Carlo simulations carefully done by Janke and Kappler[3]. What should be emphasized is that we obtained the values of the specific heat in the accuracy of about 0.1 percent at $q = 5$ where the correlation length is as large as 2500[2]. As for the asymptotic behavior of $F^{(2)}$ at $q \rightarrow 4_+$, the Padé data of $F_d^{(2)}/x$ and $F_o^{(2)}/x$ have relatively large errors of a few percent around $q = 4$, but their behaviors shown in Fig. 2 are enough to convince us that the conjecture (10) is true with

$$\alpha = 0.073 \pm 0.002. \quad (12)$$

The extension of the large- q expansion to the higher energy cumulants and the magnetization cumulants is rather straightforward and now in progress.

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Table 1: The large-q expansion coefficients $a_m^{(2)}$ for the second energy cumulant.

| m | $a_m^{(2)}$ (disordered) | $a_m^{(2)}$ (ordered) |
|-----|--------------------------|-----------------------|
| 0 | 0 | 0 |
| 1 | 2 | 0 |
| 2 | 14 | 16 |
| 3 | 26 | 34 |
| 4 | 118 | 114 |
| 5 | 250 | 254 |
| 6 | 894 | 882 |
| 7 | 1936 | 1944 |
| 8 | 6160 | 6128 |
| 9 | 13538 | 13550 |
| 10 | 39774 | 39698 |
| 11 | 88360 | 88360 |
| 12 | 245188 | 245036 |
| 13 | 547468 | 547356 |
| 14 | 1457976 | 1457784 |
| 15 | 3264012 | 3263316 |
| 16 | 8410284 | 8410596 |
| 17 | 18868858 | 18865590 |
| 18 | 47391870 | 47395762 |
| 19 | 106180532 | 106166828 |
| 20 | 261607968 | 261629456 |
| 21 | 586199668 | 586145660 |
| 22 | 1415497756 | 1415594740 |
| 23 | 3174285456 | 3174081000 |

Table 2: The specific heat for some values of q .

| q | C_d | C_o |
|-----|-----------------|-----------------|
| 5 | 2889(2) | 2886(3) |
| 6 | 205.93(3) | 205.78(3) |
| 7 | 68.738(2) | 68.513(2) |
| 8 | 36.9335(3) | 36.6235(3) |
| 9 | 24.58761(8) | 24.20344(7) |
| 10 | 18.38543(2) | 17.93780(2) |
| 12 | 12.401336(3) | 11.852175(2) |
| 15 | 8.6540358(4) | 7.9964587(2) |
| 20 | 6.13215967(2) | 5.36076877(1) |
| 30 | 4.2989934145(6) | 3.4128952554(3) |

Figure 1: An example of the cluster consisting of a single polymer that contributes to the lowest order term of the $W(l_x, l_y)$ with $l_x = 4$ and $l_y = 5$. The closed circles are the sites, and the solid lines and the crosses are the bonds connecting and disconnecting the nearest neighbor sites, respectively, in the Fortuin-Kasteleyn representation.

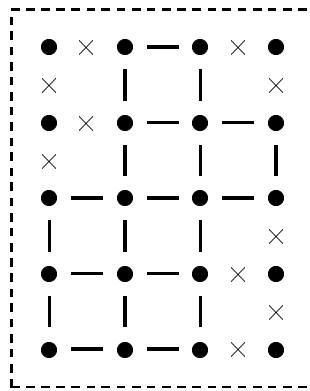


Figure 2: The ratio of the $F^{(2)}$ to x plotted versus θ . The dashed and dotted lines represent the errors for the ordered and disordered ones, respectively.

